ALCF Early Science Program

ESP Kick-Off Workshop
Project Plan Presentation

Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow

PI: Christos Frouzakis

Presenter: Paul Fischer

October 18-19, 2010

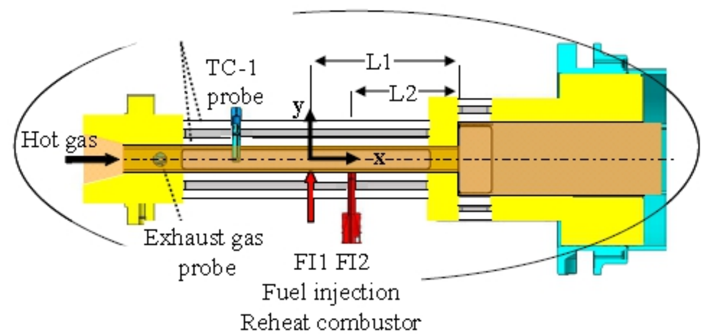
Project Overview

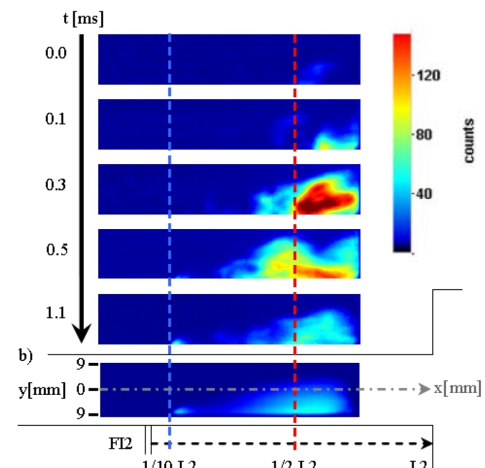
DNS of hydrogen autoignition of in a cross-flow geometry

- **Lab-scale jet in a cross flow**
- **Detailed investigation of flow and mixing**
  - parallels laboratory study in UK
- **Study conditions leading to autoignition**
- **Important for intense mixing applications**
  - Premixing ducts in lean premixed turbines
  - Mixing in reheat combustor

Scientific Field: Combustion

Codes: Nek5000



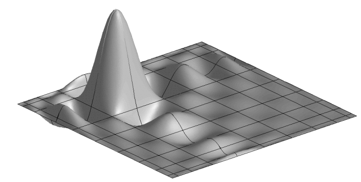


Fleck et al., ASME Turbo,2010

Numerical Code: Nek5000

http://nek5000.mcs.anl.gov *(P. Fischer, J. Lottes, S. Kerkemeier)*

- **Spatial discretization based on the spectral element method** *(Patera 1984, Devile, Fischer, Mund 2002)*
  - variational method similar to FEM using GL quadrature
  - domain partitioned into *E* quadrilateral/hexahedral elements of order *N*
  - converges exponentially fast with N for smooth solutions
  - efficient operators: memory ~ O(EN^3), work ~ O(EN^4)
  - *key kernel: small dense matrix-matrix products*



2D basis function, N=10

- **Semi-implicit time advancement**
  - Pressure & diffusive terms treated implicitly
  - Nonlinear convective terms treated explicitly
  - 2nd/3rd order characteristics methods

$$\left.\frac{\partial u}{\partial r}\right|_{\xi_i,\xi_j} = \underbrace{\sum_{p=0}^{N} \left.\frac{dh_p}{dr}\right|_{\xi_i} u_{pj}}_{mxm}$$

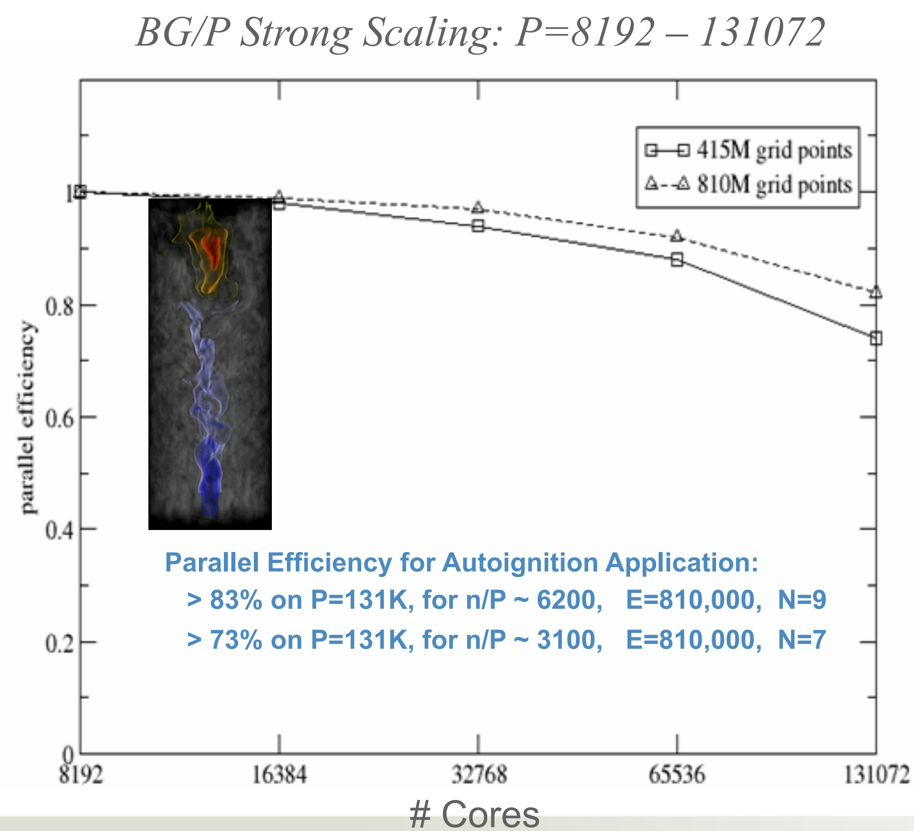
- **Physical modules**
  - Convective and conjugate transfer, MHD, free-surface flows
  - *Low Mach number combustion plugin*

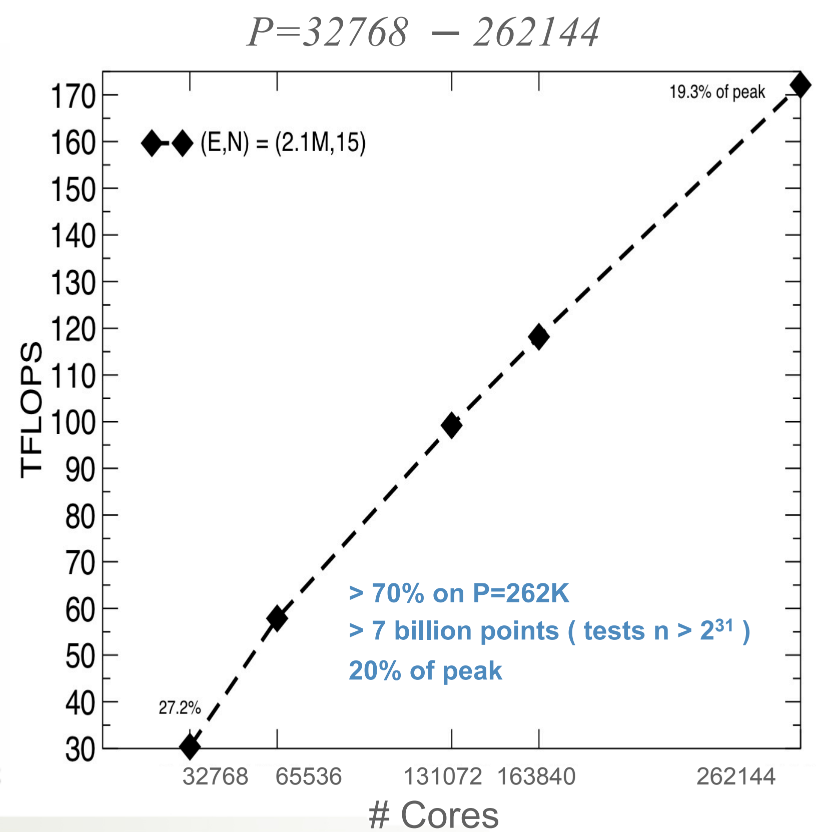
Parallelism and Existing Implementation

- **MPI everywhere**
- **Domain decomposition**
  - Recursive spectral bisection of element graph
- **Communication through scalable gather-scatter kernel, GS**
  - Topology discovery and setup in ~ .5 sec for 100 M points on 131K cores
- **Multi-level preconditioning for solvers**
  - p-multigrid for N’ = N, N/2,…,1
  - AMG for parallel coarse grid problem ~ 5% of time
  - based on optimized GS

Scaling to P=262144 Cores

- Production combustion and reactor simulations on ALCF BG/P demonstrate scaling to P=131072 with n/P ~ 3000-6,000 and η ~ .7
- Test problem with 7 billion points scales to P=262144 on Juelich BG/P with η ~ .7



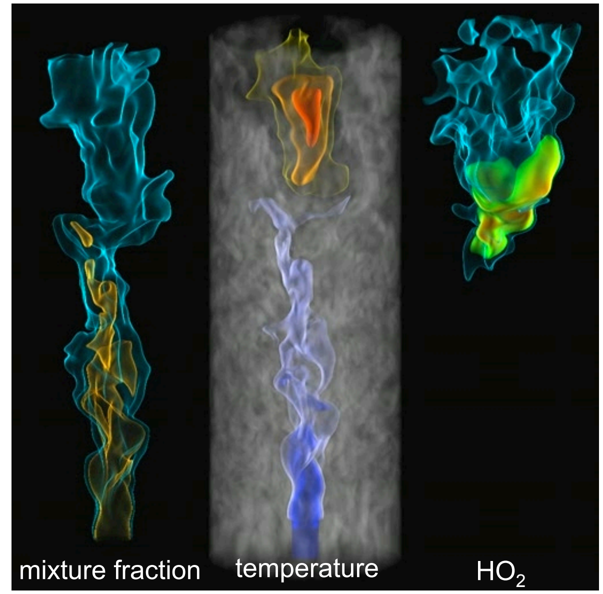


Plugin for Direct Numerical Simulation (DNS) of low Mach number reactive flows

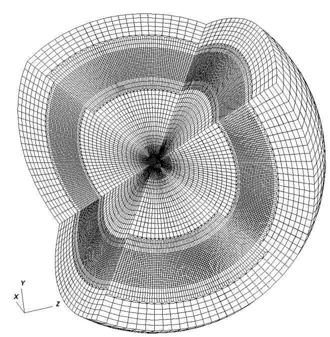
- **Low-Mach number formulation** ***(Rehm 1978, Majda 1985)***
  - hydrodynamic system can be advanced at fluid time scale
- **High-order fluid / thermochemistry splitting** ***(Tomboulides et al.,1997)***
  - optimal time integration techniques of the different subsystems
- **Adaptive BDF timestepper for thermochemistry (CVODE)**
  - efficient treatment of the non-linear coupled and stiff energy & species equations
  - Detailed chemical kinetics and transport properties
  - platform-tuned CHEMKIN compatible libraries
- **Surface kinetics**
  - conjugate heat transfer in the solid

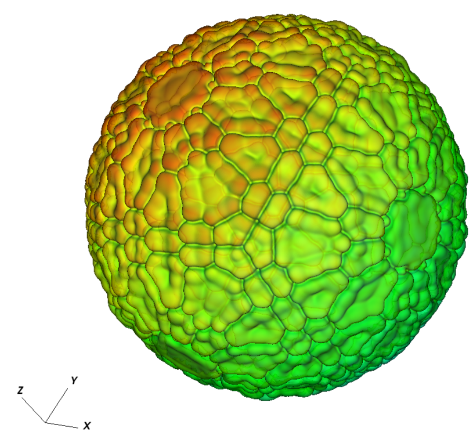
Recent DNS

- **Autoignition of a hydrogen jet in a hot turbulent co-flow**
  - Cylindrical domain: D=16mm, h=55mm
  - 300 million grid points
  - 11 ms simulated time
  - detailed H_2/O_2 mechanism (9 species / 21 rxns) and transport
  - 12M CPUh on Interpid using 32k-64k cores



- **Spherical premixed flame propagation**
  - Spherical domain
  - Locally refined grid (cubed sphere)
  - ~670 million grid points
  - 4M CPUh on Cray XT5 (Swiss National Supercomputing Center)





Library and Tool Dependencies

- **Tools**
  - High-performance dgemm optimized for small N
    - Currently using assembler written by IBM for double hummer
    - Nek data is quad-aligned (been using this trick for > 20 years)
  - Scalable MPI
    - Need to issue ~100 mpi_comm_dups (AMG)
    - Other basic functionality, but fairly conservative in MPI usage
  - VisIt (visualization)

Problem size and Anticipated Modifications for Blue Gene/Q

- **Proposed problem size**
  - 10 billion gridpoints, 100k timesteps
  - 400 μsec/gridpoint/timestep
  - Write throughput around 8 GB/s
  - I/O overhead 10%
  - *O*(120 million) Blue Gene/Q core hours
- **Ensure bounded coarse-grid-solve times for ~ $O(10^6)$ cores**
- **Add support for hardware threading. Tune kernels including**
  - Small dense matrix-matrix products [15% of time]
  - Chemical production rates and transport properties (SIMD and hardware threads) [30%]
- **Experimental support for MPI/pThread model**
  - Possibly use lightweight MPI proclet model of A. Wagner UBC

Plan for Next 6 Months Effort

- **Help find and hire a project postdoc**
  - computational scientist (CFD would be ideal)

- **Investigating "large N" kernels that will realize higher computational intensity without undue CFL constraints**

- **Identify higher level kernels amenable to threading, e.g.,**

$$\mathrm{grad}_{rst}\, u = [\ (I \times I \times D)\quad (I x D x I)\quad (D x I x I)\ ]\, u$$

$$\text{where}\ \ (I \times I \times D)\, u = \mathrm{sum}_p\, D_{ip}\, u_{pjk}\ ,\ \text{etc.}$$